10092889

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LOGINID:ssspta1613sxw

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

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| | | | |
|---|---|---|---|
| NEWS | 1 | | Web Page URLs for STN Seminar Schedule - N. America |
| NEWS | 2 | | "Ask CAS" for self-help around the clock |
| NEWS | 3 | JAN 27 | Source of Registration (SR) information in REGISTRY updated and searchable |
| NEWS | 4 | JAN 27 | A new search aid, the Company Name Thesaurus, available in CA/CAplus |
| NEWS | 5 | FEB 05 | German (DE) application and patent publication number format changes |
| NEWS | 6 | MAR 03 | MEDLINE and LMEDLINE reloaded |
| NEWS | 7 | MAR 03 | MEDLINE file segment of TOXCENTER reloaded |
| NEWS | 8 | MAR 03 | FRANCEPAT now available on STN |
| NEWS | 9 | MAR 29 | Pharmaceutical Substances (PS) now available on STN |
| NEWS | 10 | MAR 29 | WPIFV now available on STN |
| NEWS | 11 | MAR 29 | No connect hour charges in WPIFV until May 1, 2004 |
| NEWS | 12 | MAR 29 | New monthly current-awareness alert (SDI) frequency in RAPRA |
| NEWS | 13 | APR 26 | PROMT: New display field available |
| NEWS | 14 | APR 26 | IFIPAT/IFIUDB/IFICDB: New super search and display field available |
| NEWS | 15 | APR 26 | LITALERT now available on STN |
| NEWS | 16 | APR 27 | NLDB: New search and display fields available |

| | |
|---|---|
| NEWS EXPRESS | MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004 |
| NEWS HOURS | STN Operating Hours Plus Help Desk Availability |
| NEWS INTER | General Internet Information |
| NEWS LOGIN | Welcome Banner and News Items |
| NEWS PHONE | Direct Dial and Telecommunication Network Access to STN |
| NEWS WWW | CAS World Wide Web Site (general information) |

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:29:05 ON 10 MAY 2004

10092889

=> fil reg
COST IN U.S. DOLLARS

| | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 0.21 | 0.21 |

FILE 'REGISTRY' ENTERED AT 10:29:17 ON 10 MAY 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 9 MAY 2004 HIGHEST RN 680971-82-8
DICTIONARY FILE UPDATES: 9 MAY 2004 HIGHEST RN 680971-82-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

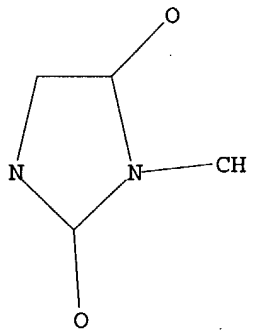
Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10092889e.str

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR

$CF_3$




Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam
SAMPLE SEARCH INITIATED 10:29:34 FILE 'REGISTRY'

10092889

SAMPLE SCREEN SEARCH COMPLETED - 112 TO ITERATE

100.0% PROCESSED 112 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1606 TO 2874
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 10:29:38 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2078 TO ITERATE

100.0% PROCESSED 2078 ITERATIONS 20 ANSWERS
SEARCH TIME: 00.00.01

L3 20 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 155.42 155.63

FILE 'CAPLUS' ENTERED AT 10:29:42 ON 10 MAY 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.


FILE COVERS 1907 - 10 May 2004 VOL 140 ISS 20
FILE LAST UPDATED: 9 May 2004 (20040509/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3 full
L4 2 L3

=> d l4 1-2 ibib abs hitstr

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:453028 CAPLUS
DOCUMENT NUMBER: 135:61331
TITLE: Preparation of 2-imidazolidinones and related compounds as selective neurokinin antagonists

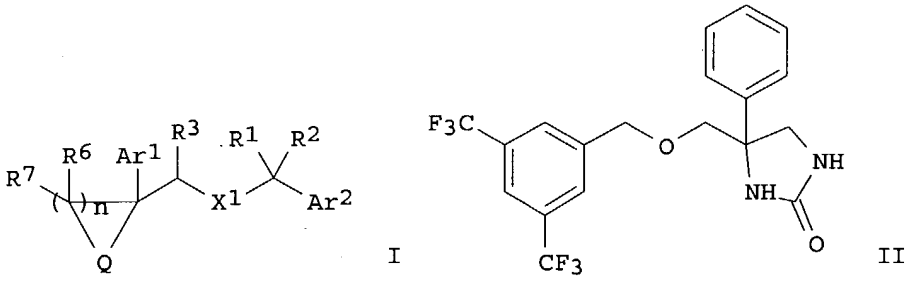
10092889

INVENTOR(S): Shih, Neng-Yang; Shue, Ho-Jane; Reichard, Gregory A.; Paliwal, Sunil; Blythin, David J.; Piwinski, John J.; Xiao, Dong; Chen, Xiao
PATENT ASSIGNEE(S): Schering Cooperation, USA
SOURCE: PCT Int. Appl., 108 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2001044200 | A2 | 20010621 | WO 2000-US33831 | 20001214 |
| WO 2001044200 | A3 | 20011213 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NO, NZ, PL, PT, RO, RU, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 6436928 | B1 | 20020820 | US 2000-737036 | 20001214 |
| US 2002123491 | A1 | 20020905 | | |
| EP 1237874 | A2 | 20020911 | EP 2000-984340 | 20001214 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL | | | | |
| JP 2003522739 | T2 | 20030729 | JP 2001-544690 | 20001214 |
| US 2003064980 | A1 | 20030403 | US 2002-163663 | 20020606 |
| US 6635630 | B2 | 20031021 | | |

PRIORITY APPLN. INFO.: US 1999-172489P P 19991217
US 2000-737036 A3 20001214
WO 2000-US33831 W 20001214

OTHER SOURCE(S): MARPAT 135:61331
GI



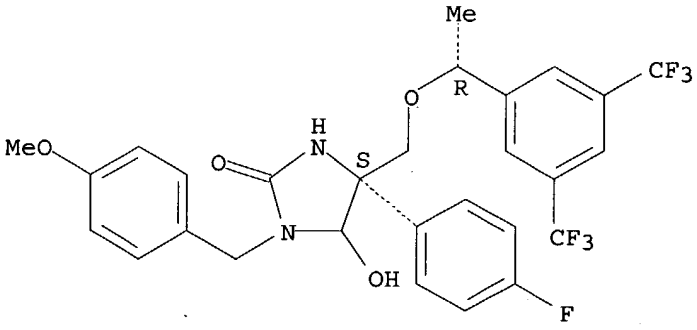

AB Title compds. [I; wherein Ar1 and Ar2 = (un)substituted heteroaryl or Ph; X1 = O, S, SO, SO2, NR12, NCOR12, or NR12SO2R15; Q = X2C(:Y)N(R4), N:C(Y1)N(R4), X2C(Y1):N, or N(R5)SO2N(R4); X2 = O, S, or NR5; Y = O, S, or NR11; Y1 = H, alkyl, SMe, alkoxycarbonylaminoalkyl, NHCOR15, or (un)substituted amino, urea, (hetero)aryl(alkyl), or heterocycloalkyl; n =

1-4; R1, R2, R3 and R7 = H, (cyclo)alkyl, CHF2, CH2F, or CF3; or R1 and R2 together with the C to which they are attached form an alkylene ring; or R1 and R2 together are :O; R4 and R12 = independently H or (cyclo)alkyl; R5 = H or (CH2)mG; m = 0-5; G = H, CF3, CHF2, CH2F, (cyclo)alkyl, (hetero)aryl, OH, (cyclo)alkoxy, SO2R13, (un)substituted amino, sulfamoyl, sulfonylamino, acylamino, carbamoyl, carboxy, urea, etc. with provisos; R6 = R7 or OH with provisos; R11 = H, (cyclo)alkyl, NO2, CN, OH, alkoxy, carbamoyl(alkyl), (hetero)aryl(alkyl), etc.; R13 = H, (cyclo)alkyl, or (hetero)aryl(alkyl), etc.; R15 = (cyclo)alkyl or CF3] were prepared as selective neurokinin antagonists. For example, cycloaddn. of (NH4)2CO3 to 2-[[3,5-bis(trifluoromethyl)phenyl]methoxy]-4'-fluoroacetophenone (4-step preparation given) afforded the 2,4-imidazolidinedione (82%), which was reduced with LAH-AlCl3 (82%). Resolution of the racemates on a chiral column, followed by recrystn., gave the imidazolidinone (-)-II. I exhibited a range of NK1 antagonist activity with Ki values ranging from about 0.1 nM to 1000 nM. Thus, I and pharmaceutical compns. of I in combination with selective serotonin reuptake inhibitors are useful in the treatment of emesis, depression, anxiety, cough, and other NK1-related disorders (no data).

IT **345579-87-5P 345580-00-9P 345580-07-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of 2-imidazolidinones and related compds. as selective neurokinin antagonists via cycloaddn. reactions)

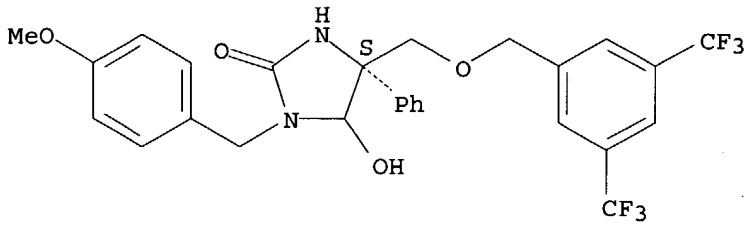
RN 345579-87-5 CAPLUS
CN 2-Imidazolidinone, 4-[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-4-(4-fluorophenyl)-5-hydroxy-1-[(4-methoxyphenyl)methyl]-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

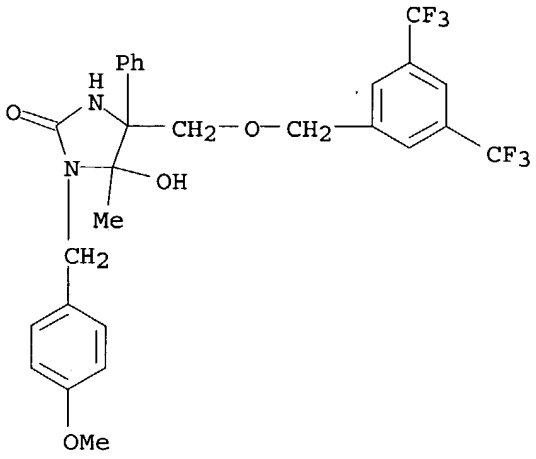



RN 345580-00-9 CAPLUS
CN 2-Imidazolidinone, 4-[[[3,5-bis(trifluoromethyl)phenyl]methoxy]methyl]-5-hydroxy-1-[(4-methoxyphenyl)methyl]-4-phenyl-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

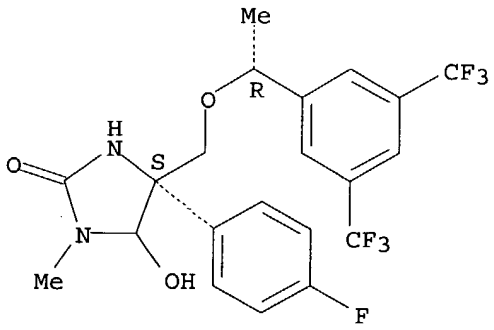


RN 345580-07-6 CAPLUS
CN 2-Imidazolidinone, 4-[[[3,5-bis(trifluoromethyl)phenyl]methoxy]methyl]-5-hydroxy-1-[(4-methoxyphenyl)methyl]-5-methyl-4-phenyl- (9CI) (CA INDEX NAME)



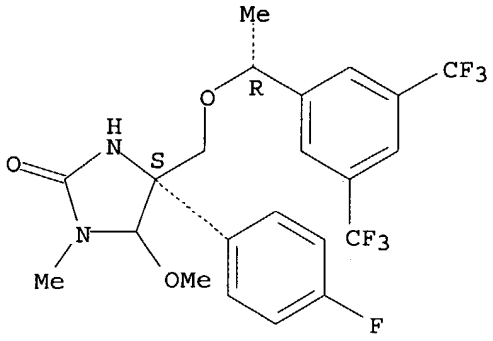
IT **345580-27-0P 345580-28-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(preparation of 2-imidazolidinones and related compds. as selective neurokinin antagonists via cycloaddn. reactions)
RN 345580-27-0 CAPLUS
CN 2-Imidazolidinone, 4-[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-4-(4-fluorophenyl)-5-hydroxy-1-methyl-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 345580-28-1 CAPLUS
CN 2-Imidazolidinone, 4-[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-4-(4-fluorophenyl)-5-methoxy-1-methyl-, (4S)- (9CI) (CA INDEX NAME)

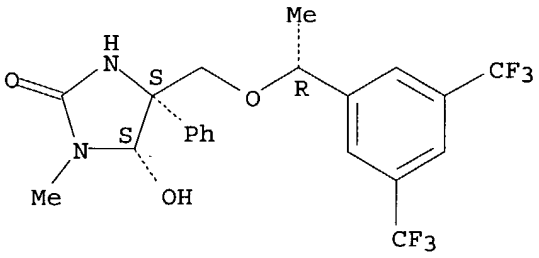
Absolute stereochemistry.




IT **345578-85-0P 345578-86-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PUR (Purification or recovery); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 2-imidazolidinones and related compds. as selective neurokinin antagonists via cycloaddn. reactions)

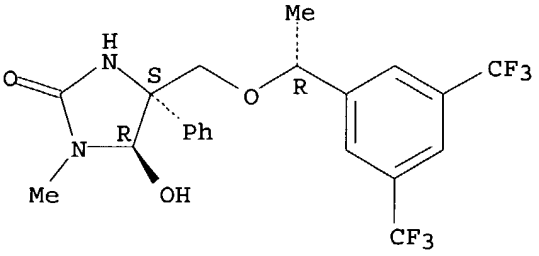
RN 345578-85-0 CAPLUS
CN 2-Imidazolidinone, 4-[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-5-hydroxy-1-methyl-4-phenyl-, (4S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




RN 345578-86-1 CAPLUS
CN 2-Imidazolidinone, 4-[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-5-hydroxy-1-methyl-4-phenyl-, (4S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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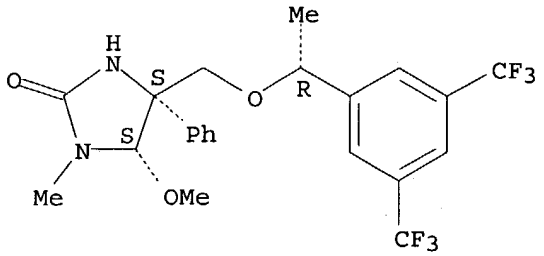
**345579-14-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-imidazolidinones and related compds. as selective neurokinin antagonists via cycloaddn. reactions)

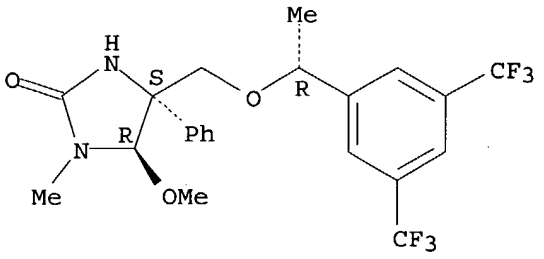
RN 345578-91-8 CAPLUS
CN 2-Imidazolidinone, 4-[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-5-methoxy-1-methyl-4-phenyl-, (4S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



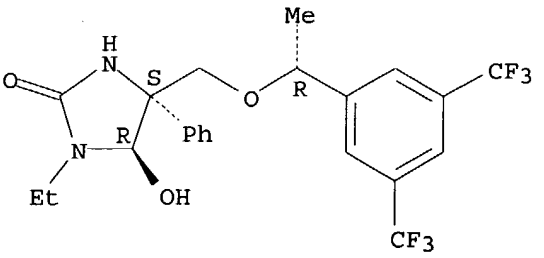

RN 345578-92-9 CAPLUS
CN 2-Imidazolidinone, 4-[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-5-methoxy-1-methyl-4-phenyl-, (4S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



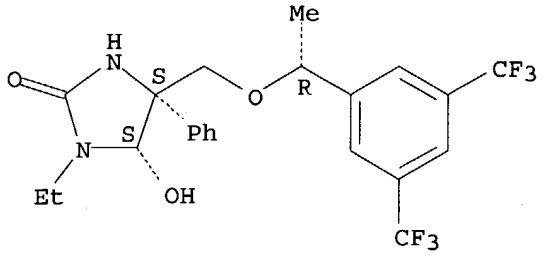

RN 345579-13-7 CAPLUS
CN 2-Imidazolidinone, 4-[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-1-ethyl-5-hydroxy-4-phenyl-, (4S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



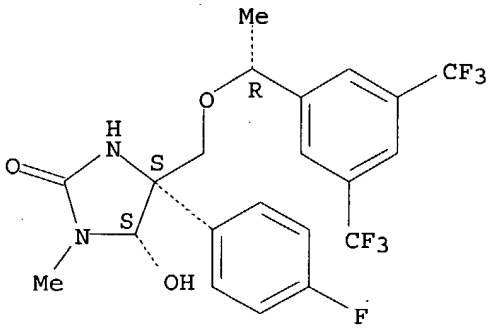
RN 345579-14-8 CAPLUS
CN 2-Imidazolidinone, 4-[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-1-ethyl-5-hydroxy-4-phenyl-, (4S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



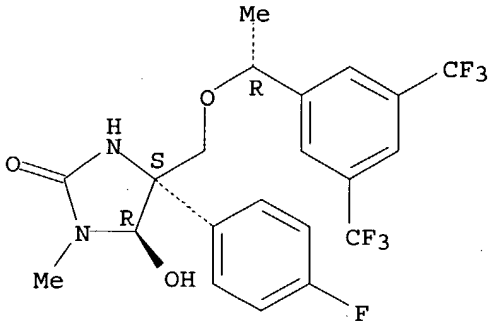
IT **345578-67-8P 345578-68-9P 345578-70-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-imidazolidinones and related compds. as selective neurokinin antagonists via cycloaddn. reactions)
RN 345578-67-8 CAPLUS
CN 2-Imidazolidinone, 4-[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-4-(4-fluorophenyl)-5-hydroxy-1-methyl-, (4S,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



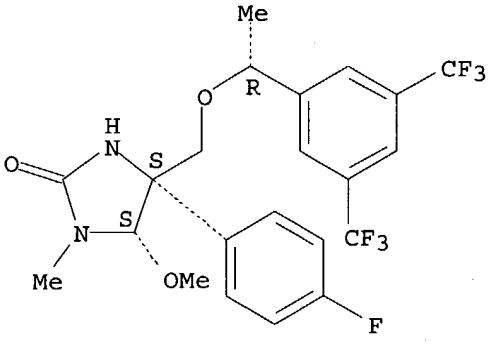
RN 345578-68-9 CAPLUS
CN 2-Imidazolidinone, 4-[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-4-(4-fluorophenyl)-5-hydroxy-1-methyl-, (4S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

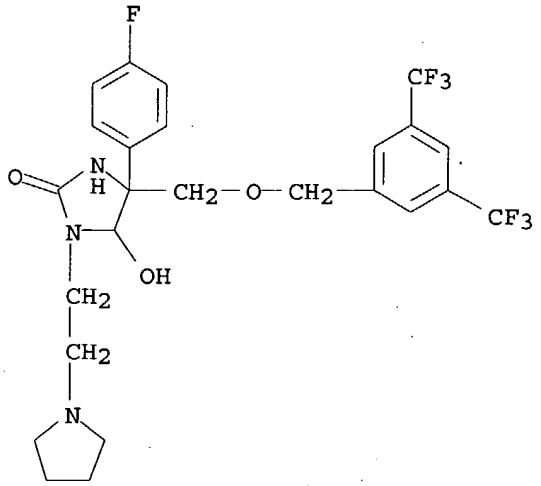


RN 345578-70-3 CAPLUS
CN 2-Imidazolidinone, 4-[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-4-(4-fluorophenyl)-5-methoxy-1-methyl-, (4S,5S)- (9CI) (CA INDEX NAME)

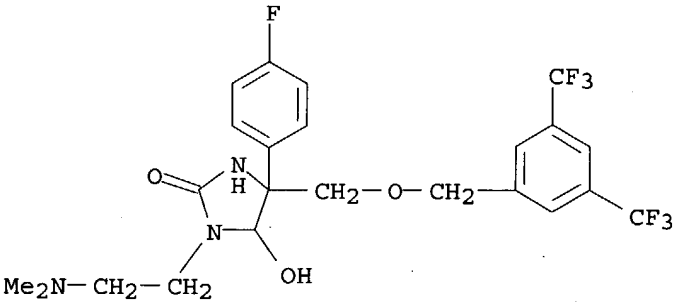
Absolute stereochemistry.



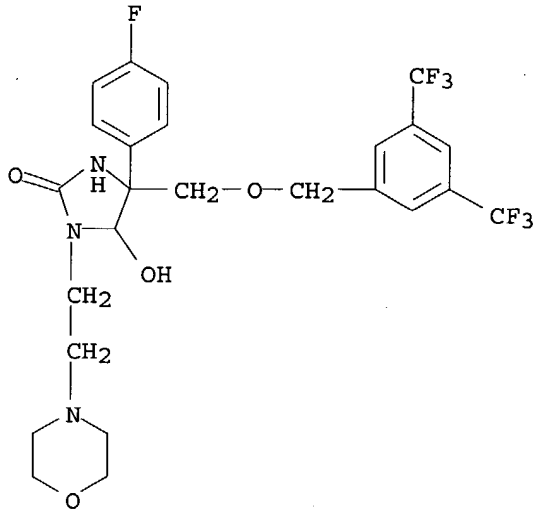
IT **345578-11-2P 345578-14-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 2-imidazolidinones and related compds. as selective neurokinin antagonists via cycloaddn. reactions)
RN 345578-11-2 CAPLUS
CN 2-Imidazolidinone, 4-[[[3,5-bis(trifluoromethyl)phenyl]methoxy]methyl]-4-(4-fluorophenyl)-5-hydroxy-1-[2-(1-pyrrolidinyl)ethyl]- (9CI) (CA INDEX NAME)



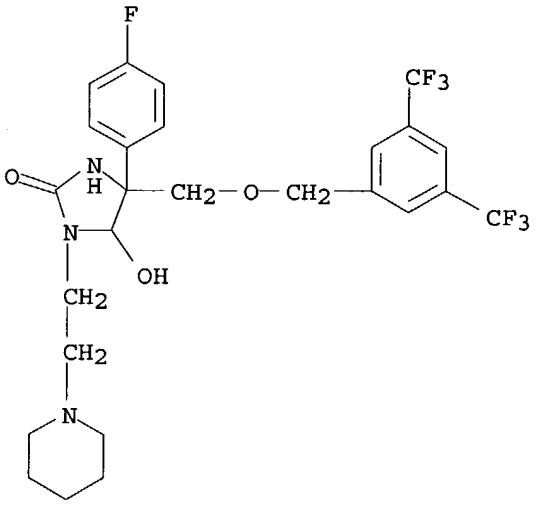
RN 345578-14-5 CAPLUS
CN 2-Imidazolidinone, 4-[[[3,5-bis(trifluoromethyl)phenyl]methoxy]methyl]-1-[2-(dimethylamino)ethyl]-4-(4-fluorophenyl)-5-hydroxy- (9CI) (CA INDEX NAME)



IT **345578-01-0P 345578-03-2P 345580-26-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2-imidazolidinones and related compds. as selective neurokinin antagonists via cycloaddn. reactions)
RN 345578-01-0 CAPLUS
CN 2-Imidazolidinone, 4-[[[3,5-bis(trifluoromethyl)phenyl]methoxy]methyl]-4-(4-fluorophenyl)-5-hydroxy-1-[2-(4-morpholinyl)ethyl]- (9CI) (CA INDEX NAME)

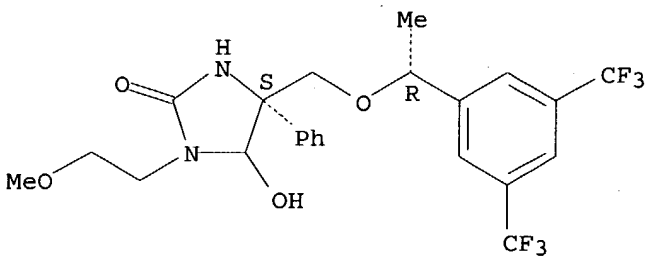


RN 345578-03-2 CAPLUS
CN 2-Imidazolidinone, 4-[[[3,5-bis(trifluoromethyl)phenyl]methoxy]methyl]-4-(4-fluorophenyl)-5-hydroxy-1-[2-(1-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)



RN 345580-26-9 CAPLUS
CN 2-Imidazolidinone, 4-[[(1R)-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]methyl]-5-hydroxy-1-(2-methoxyethyl)-4-phenyl-, (4S)- (9CI) (CA INDEX NAME)

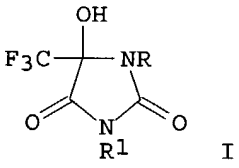
Absolute stereochemistry.



L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1987:50220 CAPLUS
DOCUMENT NUMBER: 106:50220
TITLE: 5-Hydroxy-5-(trifluoromethyl)-2,4-imidazolidinediones
INVENTOR(S): Takaoka, Akio; Ishikawa, Nobuo; Iwa, Riichi
PATENT ASSIGNEE(S): Nippon Mectron Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 61197561 | A2 | 19860901 | JP 1985-35364 | 19850226 |
| JP 05048226 | B4 | 19930720 | | |

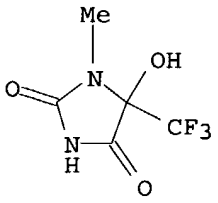
PRIORITY APPLN. INFO.: JP 1985-35364 19850226
GI



I

AB The title compds. (I; R, R1 = H, alkyl), potentially useful as virucides, neoplasm inhibitors, and herbicides, or as intermediates therefor, were prepared by reaction of trifluoropyruvic acid hydrate (II) with urea, or mono- or dialkylureas. Thus, refluxing II (prepared by autoclaving hexafluoropropylene oxide with H2O, Et2O, and silica gel) and urea in EtOH for 24 h gave 61% I (R = R1 = H).

IT **106289-13-8P**, 5-Hydroxy-5-trifluoromethyl-1-methylimidazolidine-2,4-dione
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 106289-13-8 CAPLUS
CN 2,4-Imidazolidinedione, 5-hydroxy-1-methyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)


Me
OH
N
O
CF3
N
H
O